

Chaos in Coulomb-interacting circular billiards

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We apply a molecular dynamics scheme to analyze chaotic properties of a two-dimensional circular billiard system containing two Coulomb-interacting electrons. The interaction strength is varied from the noninteracting limit with zero potential energy up to the strong-interacting regime where the relative kinetic energy approaches zero. At weak interactions the bouncing maps show jumps between quasi-regular orbits, albeit the dynamics is generally chaotic. In the strong-interaction limit we find an analytic expression for the bouncing map. Its validity in the general case is assessed by comparison with our numerical data. To obtain a quantitative view on the degree of chaoticity, we compute the escape rates that, apart from very weak interactions as well as the strong-interaction limit, suggest generally chaotic behavior that is independent of the interaction strength.

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I. INTRODUCTION

Classical billiard systems have attracted continuous interest for several decades due to their applicability to demonstrate chaotic dynamics through (semi)analytic and numerical calculations [1–3]. On the other hand, laboratory experiments on, e.g., microwave billiards [2], quantum dots [3], and more recently even graphene [4] have rapidly extended the interest in chaos across different fields in physics. Along this development, billiard systems are becoming a key element in the studies of classical and quantum chaos both theoretically and experimentally.

Most billiard studies have focused on *single-particle* properties of systems ranging from regular (integrable) to chaotic (nonintegrable) systems, including also pseudointegrable billiards [5] such as regular billiards with singular scatterers inside the system. Two-particle billiards have been studied with hard-sphere contact interactions in, e.g., rectangular [6] and mushroom-shaped [7] cavities. To the best of our knowledge, such studies with Coulomb interactions – and with the focus on classical chaotic properties – have been restricted to different two-dimensional (2D) oscillators [8–11], apart from a recent molecular-dynamics (MD) study on rectangular billiards in magnetic fields [12]. The MD scheme is a computationally efficient approach to many-particle billiards that, in principle, can be extended to large systems without compromising on the numerical complexity of the long-range Coulomb interaction. It is noteworthy that the Coulomb interaction is a physically meaningful choice when considering similar systems in, e.g., quantum-dot physics [3, 13, 14].

Here we adopt the MD approach to analyze the classical chaoticity of a 2D circular hard-wall billiards with two Coulomb-interacting electrons. The system is chosen due

to its simplicity as a prototype model for regular billiards in the *noninteracting* limit [1], and the possibility to find an approximate expression for the bouncing map in the *strong-interaction limit*. In the intermediate regime the system is expected to exhibit chaotic behavior. Due to these features the system provides a well-grounded path into examinations of both classical and quantum chaos in Coulomb-interacting billiard systems. We point out that soft billiards are better known in this respect; for example, the two-electron circular harmonic oscillator is regular and becomes mixed (partly regular, partly chaotic) if ellipticity is added in the external potential [11].

Our main tool to analyze the chaoticity in an interacting system is the escape rate. In the noninteracting case, Kolmogorov-Arnold-Moser (KAM) islands [1] and nonisolated periodic orbits with at least one Lyapunov exponent close to zero give rise to a power-law tail in the escape rate distribution. On the other hand, fully chaotic systems exhibit exponential escape rate distributions [15–19].

The paper is organized as follows. In Sec. II we briefly introduce the system and our time-propagation scheme. In Sec. III A we show bouncing maps that demonstrate clear signals of chaotic behavior through a large range of the interaction strength. At weak interactions, bouncing maps are found to jump between quasi-regular trajectories. In Sec. III B we analyze in detail the strong-interacting limit and find an approximate expression for the bouncing map. The expression agrees with the numerical result, and at weaker interactions it becomes only approximate. Finally, in Sec. III C we assess the degree of chaoticity by considering escape rates out of the system. Apart from very weak interactions, we find exponential escape in a wide range of the interaction strength. This indicates strongly uncorrelated trajectories and thus chaotic behavior. The paper is summarized in Sec. IV.

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II. SYSTEM AND METHODOLOGY

We consider two Coulomb-interacting electrons in a circular hard-wall potential. The collisions with the boundary are elastic and the system is described by the Hamiltonian

$$H = \frac{1}{2} (v_1^2 + v_2^2) + \frac{\alpha}{|\mathbf{r}_1 - \mathbf{r}_2|} \quad (1)$$

in Hartree atomic units (a.u.) ($\hbar = e = m_e = (4\pi\epsilon_0)^{-1} = 1$). Here \mathbf{r}_i is the position of the i th electron from the center of the system, and α is a parameter that determines the interaction strength. Introducing α in the numerator of the interaction term is equal to the scaling the length and time by a factor of $1/\alpha$ and keeping the numerical value of the total energy and the velocity the same. In all our simulations the total energy of the system is fixed to $E = 1$ and the radius of the circle to $R = 1/2$. The interaction strength is restricted to $0 \leq \alpha \leq 1$, where $\alpha = 0$ corresponds to noninteracting electrons, and $\alpha = 1$ corresponds to electrons being localized at the opposite sides of the circle with zero motion.

To propagate the electrons we use molecular dynamics with the velocity Verlet [20] algorithm. The positions and velocities of each electron are calculated from

$$\mathbf{r}(t + \Delta t) = \mathbf{r}(t) + \mathbf{v}(t)\Delta t + \frac{1}{2}\mathbf{a}(t)\Delta t^2; \quad (2)$$

$$\mathbf{v}(t + \Delta t/2) = \mathbf{v}(t) + \frac{1}{2}\mathbf{a}(t)\Delta t; \quad (3)$$

$$\mathbf{a}(t + \Delta t) = \sum_i \mathbf{F}_i[\mathbf{r}(t + \Delta t)]; \quad (4)$$

$$\mathbf{v}(t + \Delta t) = \mathbf{v}(t + \Delta t/2) + \frac{1}{2}\mathbf{a}(t + \Delta t)\Delta t. \quad (5)$$

We define θ and s as the generalized coordinates describing the collisions with the boundary. θ is the angle between the velocity vector of the incoming electron and the tangent of the boundary, so that $\theta < \pi/2$ and $\theta > \pi/2$ correspond to counterclockwise and clockwise traveling directions, respectively. Here $s \in [-\pi/2, \pi/2]$ is the oriented arc length from the chosen origin.

III. RESULTS

A. Bouncing maps

In Fig. 1 we show examples of bouncing maps and electron trajectories for a two-electron circular billiard with different interaction strengths α . In this case the bouncing maps consist of 14 000 ($\alpha = 10^{-5}$) and 5500 ($\alpha = 0.2$ and 0.7) collisions with the boundary. The noninteracting circular system with $\alpha = 0$ is a well-known example of regular billiards [1] represented by straight lines in the map (constant bouncing angle) and straight trajectories forming a star-shaped pattern, where the inner part of the circle remains empty. When $\alpha = 10^{-5}$ we

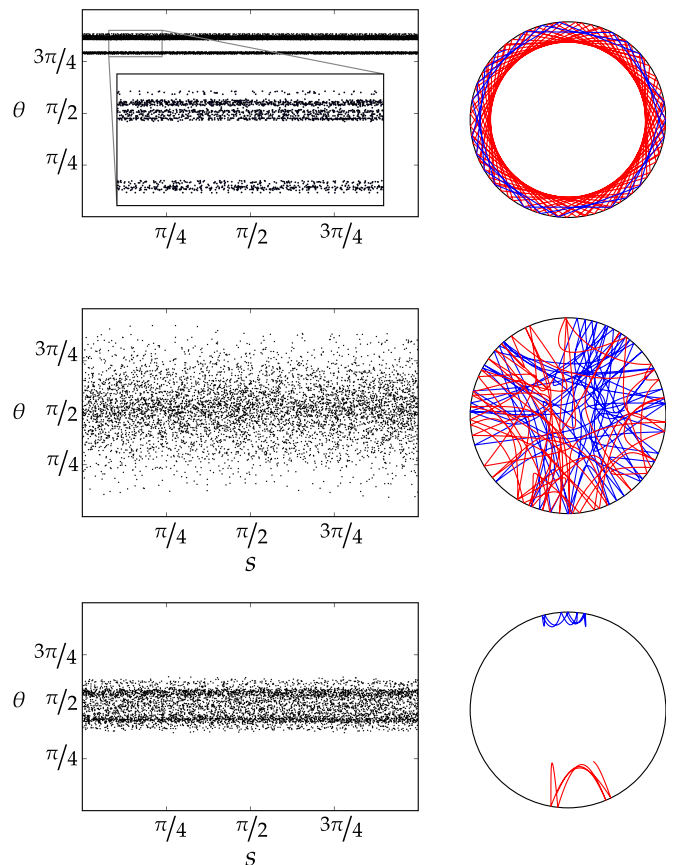


FIG. 1: Examples of bouncing maps (of one of the electrons) and trajectories for a two-electron circular billiards with different interaction strengths: $\alpha = 10^{-5}$ (up), $\alpha = 0.2$ (middle), $\alpha = 0.7$ (bottom). Only a small section of the trajectories corresponding to the bouncing maps are shown.

find emerging deviations from this limit as visualized in the inset of the upper panel of Fig. 1. When the electrons pass each other the interaction is pronounced and we may find “jumps” from one quasi-regular trajectory to another one (close-lying parallel lines in the inset).

In the intermediate-interaction range (middle panel of Fig. 1) the chaoticity of the system is clear, so that the bouncing map rapidly becomes completely filled. As expected, the distribution of the bouncing map is centered at $\theta = \pi/2$, so that, *on the average*, the electrons hit the boundary along the normal vector.

If α is increased above $\alpha \sim 0.5$ we find that for some trajectories the maximum of the probability distribution for θ splits into two. This is visible in the bottom panel in Fig. 1 for $\alpha = 0.7$. However, the splitting is smoothed out when a large ensemble of trajectories is taken into account. When α is increased further, the system gradually becomes (quasi)regular and eventually the bouncing map reduces into a one-dimensional curve. In the following we carry out analytic calculations in the strong-interaction limit.

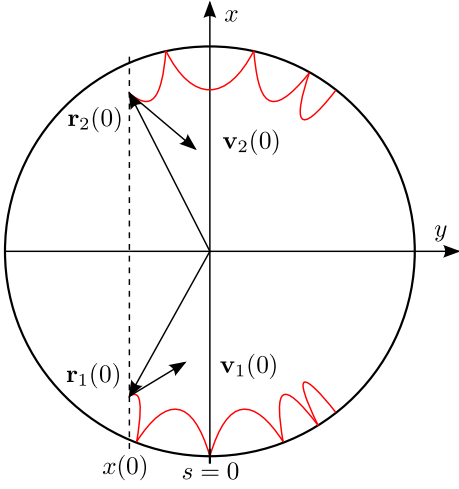


FIG. 2: Two electrons oscillating at the opposite sides of the circle when the interaction is strong ($\alpha \gtrsim 0.9$). The initial positions and velocities are shown.

B. Strong-interaction limit

In the strong-interaction limit $\alpha \rightarrow 1$, the two-electron dynamics shows regular characteristics. The electrons are confined at opposite sides of the circle as visualized in Fig. 2. Here we focus on the special case with total angular momentum $L = 0$ which is conserved due to the rotational symmetry. Hence, according to the choice of coordinate axes in Fig. 2 we may approximate $x \equiv r_{1,x} \approx r_{2,x}$. We point out, however, that the y coordinate does not have mirror-symmetry in the general case. Note also the position of $s = 0$ at $x = 0$ in Fig. 2, so that $s \in [-s_{\max}, s_{\max}]$.

As the second approximation, the electron velocity perpendicular to the edge, v_{\perp} , can be taken as a constant, i.e., it is approximately the same for all possible values of s . After straightforward geometrical analysis, taking into account the conservation of E and L , we can calculate the tangential velocity $v_{\parallel}(s)$ and further the bouncing angle from $\tan \theta = v_{\perp}/v_{\parallel}$. Thus, we obtain the following strong-interaction approximation for the bouncing map of electron 1:

$$\theta_1(s) = \arctan \sqrt{\frac{2K_0 + 2U_0 - 2U_a - L_{1,0}^2/R^2}{U_b - U_c(s) + L_{1,0}^2/R^2}}, \quad (6)$$

where $K_0 = v_{1,x}^2(0) + v_{1,y}^2(0)$ is the initial kinetic energy of the electron, $L_{1,0} = x(0)v_{1,y}(0) - y_1(0)v_{1,x}(0)$ is its initial angular momentum (note that $x = x_1 \approx x_2$ according to our approximation above), $U_0 = \alpha/[|y_1(0)| + |y_2(0)|]$ is the initial potential energy, and $R = 1/2$ is the radius of the circle. Furthermore, Eq. (6) has three potential energy components corresponding to situations, where electron 1 touches the boundary at $t = 0$, both electrons touch the boundary at $t = 0$, and both electrons touch the boundary at s time t . These components, respec-

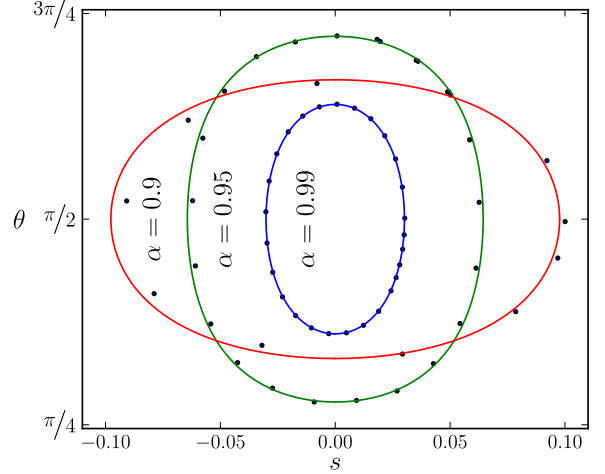


FIG. 3: Analytic result for the large- α limit [Eq. (6)] of the bouncing map (solid lines) for $\alpha = 0.99, 0.95$, and 0.9 . The corresponding simulated, i.e., numerically exact values are shown by points.

tively, have expressions

$$U_a = \frac{\alpha}{|y_2(0)| + \sqrt{R^2 - x(0)^2}}, \quad (7)$$

$$U_b = \frac{\alpha}{2\sqrt{R^2 - x(0)^2}}, \quad (8)$$

$$U_c(s) = \frac{\alpha}{2R \cos(s/R)}. \quad (9)$$

Figure 3 shows the results from Eq. (6) for $\alpha = 0.99, 0.95$, and 0.9 (solid lines). The *simulated*, i.e., the numerically exact values, are shown by points. As α is decreased we find gradual deviation from the simulated data. At $\alpha = 0.9$ the deviation is already clearly visible. We may thus state that Eq. (6) provides a reasonable approximation for the bouncing map at $\alpha \gtrsim 0.9$. This threshold slightly depends on the initial conditions; the examples in Fig. 3 are chosen such that the deviations between the analytic expression and the numerical data are large.

C. Escape rates

A natural sign of chaos in a general N -electron system is the loss of autocorrelation of the trajectory. In the present eight-dimensional phase space this is tedious to calculate from a single trajectory, and naturally even more difficult over all the trajectories in order to perform statistical averaging. However, we can analyze the chaoticity of our system indirectly by calculating the *escape rates* through a hole on the billiard boundary as a function of α . In the single-electron case, systems with KAM islands or nonisolated and nonhyperbolic orbits have a power-law tail in the escape-rate distributions as a function of time or number of collisions with the

boundary [15–19]. In contrast, in fully chaotic systems the distribution is exponential.

We set 10 holes in the boundary covering together $1/50$ of the boundary length – the same fraction as in Ref. [19]. The escape rates are considered as a function of the total number of collisions rather than the propagation time, since the characteristic time scale strongly depends on the interaction strength α . For each α we compute $2.5 \dots 6 \times 10^5$ respective trajectories with random initial conditions and store the number of boundary collisions before the escape. The time steps are chosen in the range $\Delta t = 10^{-8} \dots 10^{-7}$, so that the convergence is ensured in every calculation, while the numerical efficiency is maximized.

Figure 4(a) shows the resulting histograms of the escape-rate calculations. First, the noninteracting situation ($\alpha = 0$) has a clear power-law tail with $P(n) \propto n^{-\gamma} + \text{const}$, where $\gamma \approx 3.46$. In contrast, when $0.1 \leq \alpha \leq 0.5$ an excellent fit to the exponential behavior with $P(n) = 49^{n-1}/50^n$ (straight line) can be found. This relation results from the system geometry: each collision has the escape probability of $1/50$, and thus for the n :th collision to lead to escape we find $P(n) = (49/50)^{n-1}(1/50)$. This essentially means that the correlation with two successive bounces is completely lost, and hence the system can be classified as chaotic.

In Fig. 4(b) we have a closer look to the weak-interaction limit with $\alpha = 10^{-6}$. A good fit to the computed data is obtained with a power-law curve having $\gamma \approx 4.08$, i.e., the escape is slightly faster than in the noninteracting limit. However, at small time scales the behavior is very similar to the $\alpha = 0$ as the trajectories essentially follow the same (quasi-)regular patterns. These quasi-stable trajectories also give arise to power-law tail in the escape-rate distributions for weak interactions. However, the interaction reduces the lengths of the quasi-regular parts of the electron trajectories and thus decreases the survival probability (and escape rates) at longer time scales.

Concluding, our results on the escape probabilities show that the transition to exponential escape rates – and thus to chaotic behavior – is (i) smooth (not abrupt as a function of α), (ii) it occurs first at large times (large number of collisions) in the histogram, and (iii) it generally appears at relatively small values for α . Our tests indicate that at $\alpha \sim 10^{-3}$ the most part of the calculated escape-rate histogram is closer to an exponential behavior than to the power-law one. We point out that the large- α regime is excluded in this analysis due to numerical reasons: at $\alpha > 0.5$ we would need to decrease the holes due to small-scale motion close to the boundary, and thus the time step should be decreased as well. Hence, for consistency of the results we have focused here only on the range $0 \leq \alpha < 0.5$.

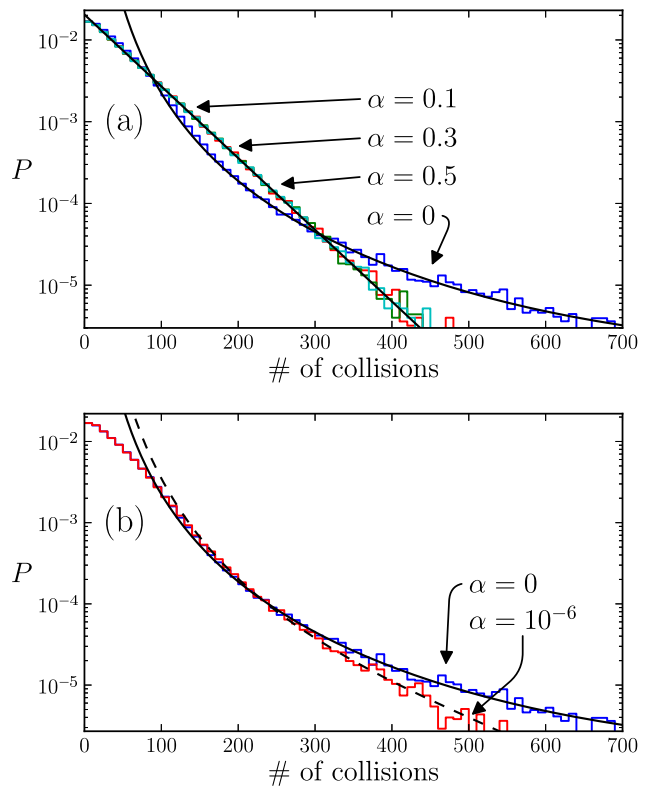


FIG. 4: (a) Histograms of the escape rates in a two-electron circular billiard. The noninteracting case shows power-law behavior in the tail (curved solid line), whereas at $0.1 \leq \alpha \leq 0.5$ the escape rate is exponential (straight solid line). (b) At very weak interactions $\alpha = 10^{-6}$ we find a mixture of these tendencies due to quasi-regular trajectories in the system.

IV. SUMMARY

To summarize, we have made a thorough look into chaotic dynamics of circular billiards containing two Coulomb-interacting electrons with the full range of interaction strengths ($0 \leq \alpha \leq 1$). Close to both weak- and strong-interaction limits the bouncing maps show traces of quasi-regular behavior, although the dynamics generally appears as chaotic. In the strong-interaction limit we are able to find an analytic expression for the bouncing map that agrees very well with the calculated data at $\alpha \rightarrow 1$. At smaller α the predictive power of the expression reduces, although the agreement is reasonable down to $\alpha \sim 0.9$. To assess the chaoticity we have calculated escape rates as a function of α and found similar exponential behavior through a wide range of interaction strengths, which indicates chaotic behavior. As the circular billiard is completely regular in the noninteracting limit, our finding suggests universally chaotic behavior in Coulomb-interacting billiards with hard walls. This expected generality is a natural subject of future studies.

Acknowledgments

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